

# Scattering quantum circuit to measure Bell's time inequality violation: a NMR demonstration using maximally mixed states

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**Abstract.** In 1985 A.J. Leggett and A. Garg proposed a Bell-like inequality to test the (in)compatibility between quantum mechanics the two fundamental concepts. The first concept is the “macroscopic realism”, that is, the quality of a physical property of a quantum system to be independent of observation at the macroscopic level, and the second concept is the “noninvasive measurability”, that is, the possibility of performing a measurement without disturbing the subsequent evolution of a system. One of the key requirements for testing the violation of the Leggett-Garg inequality, or time Bell's inequality, is the ability to perform non-invasive measurements over a qubit state. In this paper we present a quantum scattering circuit which implements such a measurement for maximally mixed states. The operation of the circuit is demonstrated using liquid-state NMR in Chloroform, in which the time correlations of one-qubit is measured on a probe (ancillary) qubit state. The results show clearly a violation region, and are in excellent agreement with the quantum mechanical predictions.

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It has been recently reported by Palacios-Laloy and co-workers [1] an experimental demonstration of Bell's time inequality violation in superconductors, which is the first experimental test of the original proposal made by Leggett and Garg in 1985 [2]. Experiments of this kind are extremely important to test the foundations of quantum mechanics. The fundamental ideas addressed in the Leggett-Garg proposal were the "macroscopic realism" and "noninvasive measurability at the macroscopic level". The former is the assumption that physical properties are independent of observation at macroscopic level. The later condition implies the existence of measurements which can determine the state of a macroscopic system introducing an arbitrarily small perturbation that does not affect the subsequent dynamics. Studying these ideas on the superconducting current in a SQUID (Superconducting Quantum Inference Device) the authors conclude that quantum mechanics is incompatible with these two assumptions. Besides that, Leggett-Garg inequality has also been related to the quantuness of computational algorithms [3] and the outcome of operators weakly measured [4, 5, 6], the so called weak values [7]. In particular, the reference [4] has shown that strange weak values, those values which exceed the range of eigenvalues associated to the observable in question, can only be found if and only if a Leggett-Garg inequality is violated.

On its usual form, Bell's inequality is violated by multipartite quantum systems sharing an entangled state. Given a pure entangled state, it is always possible to find a kind of inequality based on local realism which is violated by quantum mechanics. However, it is important to notice that some entangled mixed states do not violate standard Bell's inequalities, unless additional local actions with classical communication and post-selection (rejecting part of the original ensemble) are performed [8]. On another hand, a recent work [9], has suggested that quantum entanglement can be produced between thermal states with nearly maximum Bell-inequality violation, even when the temperatures of both systems approach infinity.

On the practical side, entanglement has been recognized as a key ingredient for quantum computation and quantum communication [10], and violation of Bell's inequality can be used as a criterion of efficiency for quantum communication protocols [11, 12]. Moreover, whereas multipartite quantum systems can exhibit non-local correlations introduced by entanglement, one single quantum object, like a spin-1/2 particle, can exhibit non-classical *time-correlations* such as those addressed in the Leggett-Garg paper. In order to observe such quantum time correlations during the evolution of a qubit and test the inequality, it is necessary to perform the a noninvasive measurements. This restriction imposes serious experimental difficulties.

The idea of Leggett-Garg is to measure time correlation functions of an observable  $\mathcal{O}$  (which has eigenvalues  $\pm 1$ ),  $C_{k,m} = \langle \mathcal{O}(t_k) \mathcal{O}(t_m) \rangle$ , at different instants of time,  $t_k$  and  $t_m$ , during which the system evolves under the action of a time-independent Hamiltonian,  $\mathcal{H}$ , according to the Schroedinger equation  $|\psi(t)\rangle = \exp(-i\mathcal{H}t/\hbar) |\psi(0)\rangle$  ( $|\psi(0)\rangle = |\psi(t=0)\rangle = |\psi_0\rangle$ ).

The Leggett-Garg inequality, of the Wigner type [13], states that for some chosen

set of three different instants of time,  $t_1 < t_2 < t_3$ , macroscopic realism imposes that:

$$K \equiv C_{1,2} + C_{2,3} - C_{1,3} \leq 1 \quad (1)$$

The condition for observing violations of this inequality, as demonstrated by Kofler and Brukner [13], is that the initial state of the system,  $|\psi_0\rangle$ , cannot be an eigenvector of  $\mathcal{H}$ . The dichotomic observable  $\mathcal{O}$  is then defined in terms of the initial state as  $\mathcal{O} \equiv 2|\psi_0\rangle\langle\psi_0| - \mathcal{I}$ , being  $\mathcal{I}$  the identity matrix. Under time evolution, a measurement of this observable,  $M(\mathcal{O})$ , will indicate whether the system is still in  $|\psi_0\rangle$  ( $M(\mathcal{O}) = +1$ ), or not ( $M(\mathcal{O}) = -1$ ). Performing measurements for three different times such as  $t_2 - t_1 = t_3 - t_2 = \Delta t$ , the inequality (1) takes the form [13]:

$$K = 2 \cos\left(\frac{\Delta E \Delta t}{\hbar}\right) - \cos\left(2\frac{\Delta E \Delta t}{\hbar}\right) \leq 1 \quad (2)$$

where  $\Delta E$  is the energy separation between the qubit eigenvalues. This inequality is clearly violated for  $0 < \Delta E \Delta t / \hbar < \pi/2$ , and is maximally violated for  $\Delta E \Delta t / \hbar = \pi/3$ .

A great deal of effort has been put, since the work of Leggett-Garg [2], to find ways to implement non-invasive measurements [14, 15, 16, 17] and verify the violation of the inequality (1). In particular, the proposal of *weak measurements* of [15] has been implemented on the experiment of Palacios-Laloy [1]. On spite of the successful demonstration of Bell's time inequality violation in [1], the literature still lacks an example of a full quantum protocol with noninvasive measurements. The proposal of this paper is to present an scattering quantum circuit based on [13] which performs such a test for a maximally mixed state, and to demonstrate its implementation using the well established NMR quantum information processing experimental techniques [18, 19].

The circuit proposed in this paper correlates a single microscopic qubit (ancillary), to a quantum ensemble at infinite temperature. This is similar to the quantum Schrödinger's cat paradox, where the macroscopic "cat" corresponds to a thermal state at infinite temperature, a state that is often believed to not exhibit quantum properties. The ancillary qubit probes the time correlations of the ensemble without disturbing its subsequent dynamics.

An early example of NMR application to a quantum scattering circuit appeared on a paper by Miquel et al., [20] in the context of measuring Wigner functions on phase-space using NMR on liquid Trichloroethylene, a well known 3-qubit system. On a scattering circuit, a probe qubit (ancillary), prepared in a known initial state, interacts with the system in such a way that a measurement over its state after the interaction brings information about the system state. For this, it is necessary that: (i) the input state of the probing qubit to be known, and (ii) that the interaction can be controlled. Figure 2 shows a scattering circuit to obtain time correlation function of a qubit by measuring the state of the probing qubit, which interacts with it. For a non-invasive measurement, it is necessary to prepare the system input state in such a way that the controlled interaction does not affect it. Such a state can be worked out as follows: consider the input state,

$$\rho_{in} = \rho_{probe} \otimes \rho_{sys} = |0\rangle\langle 0| \otimes |\psi_0\rangle\langle\psi_0| \quad (3)$$

where the first qubit on the left is the probe, entering the circuit on  $|0\rangle$ , and the other one is the system, prepared in the state  $|\psi_0\rangle$ . Upon the transformations shown on Figure 2, the output of the scattering circuit will be [20]:

$$\rho_{out} = |\varphi\rangle\langle\varphi| \quad (4)$$

where  $|\varphi\rangle = |0\rangle\otimes(\mathcal{I} + U)|\psi_0\rangle + |1\rangle\otimes(\mathcal{I} - U)|\psi_0\rangle$ , being  $U = e^{i\mathcal{H}t_m/\hbar}\mathcal{O}e^{-i\mathcal{H}t_m/\hbar}e^{i\mathcal{H}t_k/\hbar}\mathcal{O}e^{-i\mathcal{H}t_k/\hbar}$ . The real part of the expected value of the spin  $z$ -component for the probing qubit is:  $\langle\sigma_z\rangle = \text{Tr}\{\rho_{sys}U\}$  and therefore:

$$\langle\sigma_z\rangle = \langle\psi_0|e^{i\mathcal{H}t_m/\hbar}\mathcal{O}e^{-i\mathcal{H}t_m/\hbar}e^{i\mathcal{H}t_k/\hbar}\mathcal{O}e^{-i\mathcal{H}t_k/\hbar}|\psi_0\rangle \quad (5)$$

which implies that:

$$\langle\sigma_z\rangle = \langle\mathcal{O}(t_m)\mathcal{O}(t_k)\rangle \quad (6)$$

According to [13], any combination of two states which are orthogonal to the eigenvectors of  $\mathcal{H}$  will lead to the violation of the inequality (1). Thus, both states  $|0\rangle$  and  $|1\rangle$  will lead to a violation when choosing  $\mathcal{H} = \hbar\omega\sigma_x$ , being  $\sigma_x$ , one of the Pauli matrices. It is interesting to note that the theoretical prediction of the quantity  $K$ , defined in (1), as a function of  $\Delta t$  is identical for both states and is given by the Equation (2). Therefore, any statistical mixture of those states,  $p_0|0\rangle\langle 0| + p_1|1\rangle\langle 1|$ , will also violate the same inequality. Although the violation of Leggett-Garg Inequality does not depend on the degree of mixedness, most states cannot be used in a experimental test using the scheme proposed here because the application of the circuit of Figure 2 in a general state will not perform a noninvasive measurement. Only the completely mixed state ( $p_0 = p_1 = 1/2$ ) does not undergo any change during the application of the circuit. Hence, this particular state is ideal for a macroscopic realism test. The probe qubit, however, is initialized on a pure state. This situation corresponds to the model of computation known as deterministic quantum computation with one quantum bit (DQC1) [21].

The ability of Nuclear Magnetic Resonance to generate quantum states and unitary transformations of quantum circuits, is well established in the literature [19, 20]. To implement the circuit of Fig 2 and demonstrate our proposal, we used a well known two-qubit NMR quantum processor: the Chloroform molecule,  $\text{CHCl}_3$ . A liquid sample of 99.99% Carbon labeled diluted in deuterated acetone was used. The experiment was performed at room temperature, in a Varian 500 MHz Shielded NMR spectrometer. It is worth noticing that the entire protocol lasts about 10 ms, whereas the characteristic decoherence time for this system is  $T_2 \approx 3$  s for Hydrogen and  $T_2 \approx 0.8$  s for Carbon. Therefore, decoherence can be neglected during the application of the protocol.

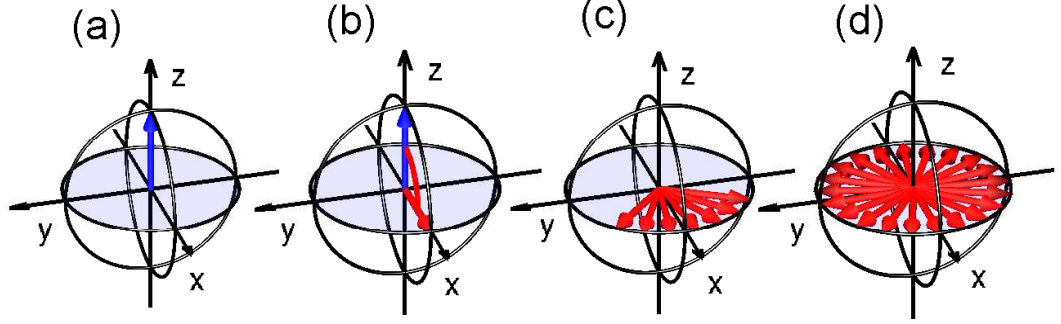
In order to observe time correlations and the violation of the inequality (1) we have used the Hamiltonian  $\mathcal{H} = \hbar\omega\sigma_x$ . In NMR, this Hamiltonian is simply implemented by radio-frequency pulses applied on the resonance of the qubit spins. The tested ensemble corresponds to an ensemble of nuclear spins  $1/2$  in a maximally mixed state, produced by a single  $\pi/2$  pulse, followed by a field gradient, as illustrated in figure 1. Due to the low

polarization of the nuclear spins at room temperature, the probe qubit is not initialized in a pure state but rather in the pseudo-pure state  $(1 - \epsilon)\mathcal{I}/2 + \epsilon|0\rangle\langle 0|$ . Since  $(1 - \epsilon)\mathcal{I}/2$  is not observed, the probe qubit in such a mixed state produces the same result as it would be observed if the probe were in a pure state and the detection efficiency of the measurement apparatus were  $\epsilon$ . The data analysis here is analog to the post-selecting procedure, used in experiments with low efficiency detection [8]. In NMR, post-selection is accomplished by normalizing the signal to a reference.

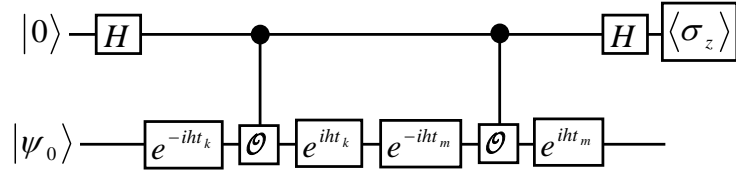
Figure 3 shows the quantum state tomography of the system input deviation density matrix  $\Delta\rho = |0\rangle\langle 0| \otimes \mathcal{I}/2 - \mathcal{I}/4$ . Figure 4 shows the correlation functions  $C_{12}$  (3a),  $C_{23}$  (3b) and  $C_{13}$  (3c) and the quantity  $K$ , defined in Eq. (1), is shown in the Figure 5. The continuous line is the quantum mechanical prediction. The results show clearly a violation region, and are in excellent agreement with the quantum mechanical predictions. However, the need of a normalization, or post-selection procedure, introduces a detection loophole [8], and thus the violation of realism can only be assumed upon the fair sampling hypothesis, i.e. the hypothesis that sample of detected events is representative of the entire system. Most of experiments testing standard Bell's inequalities are run under this assumption. The remarkable fact about NMR is that the low spin polarization implies the existence of a local and realistic hidden variable model [22, 23]. On the other hand, one must notice that truly quantum correlations can be present between the probe and the tested ensemble [24, 25].

NMR has been extremely useful for testing fundamental ideas on quantum information. In particular, studies of entanglement and fundamental quantum mechanics has been exploited in various NMR works (see for example [23, 26, 27]). Much less exploited than multipartite entangled states are the time quantum correlations proposed by Leggett and Garg. Understanding such correlations is of great relevance for fundamental physics as well for quantum computation and communication. From an experimental point of view, testing time correlations is simpler, because it can be done over one single qubit.

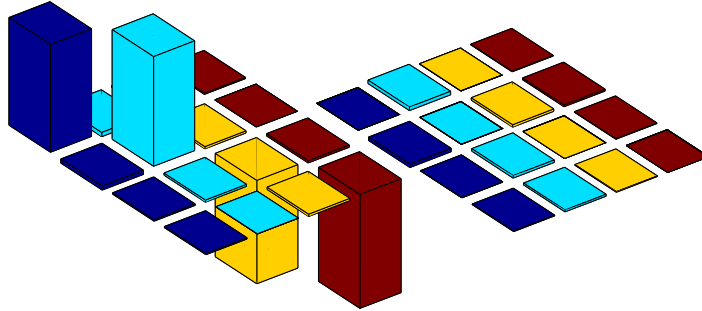
In conclusion, the results shown on this paper reveals that even in the extreme situation of a maximally mixed state, time quantum correlations persists. We have proposed, and demonstrated with a NMR quantum information processor, a scheme based on a microscopic qubit probe to test time Bell's inequalities of quantum ensembles in a maximally mixed state. Such a scheme could be useful to be implemented in recent experimental setups [9, 28] where a thermal state can be correlated to pure microscopic qubits. It is tempting to associate our results to the power of one qubit computation [21, 29, 24], and this is certainly a subject worth pursuing in further experiments. Finally, we would like to mention that the scattering quantum circuit presented here can be easily adapted to measure the three correlation functions simultaneously, using more ancillary qubits.



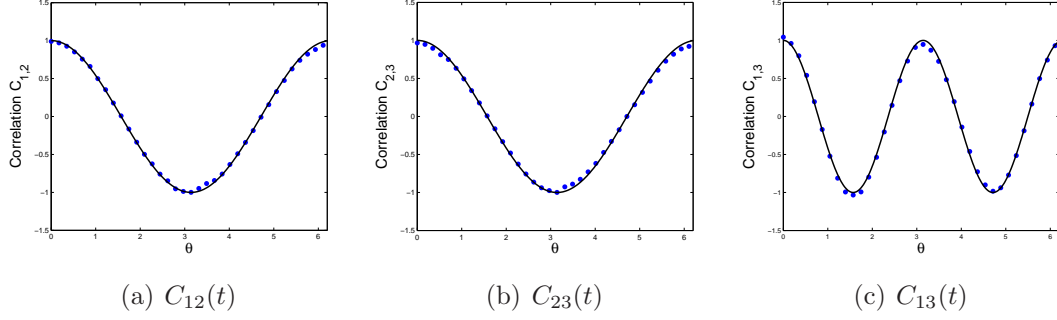
**Figure 1.** Evolution of the spins in the preparation of a maximally mixed state. (a) The Bloch vector of the spins are initially prepared in the state  $|0\rangle$  (b) A  $\pi/2$  rotation takes the Bloch vector from the state  $|0\rangle$  to the  $xy$  plane. (c) A field gradient is applied, since the field varies along the  $z$ -axis, spins in different positions in the sample start to precess with different angular velocities. (d) After some time the distribution of Bloch vectors are completely randomized, corresponding to a maximally mixed state.



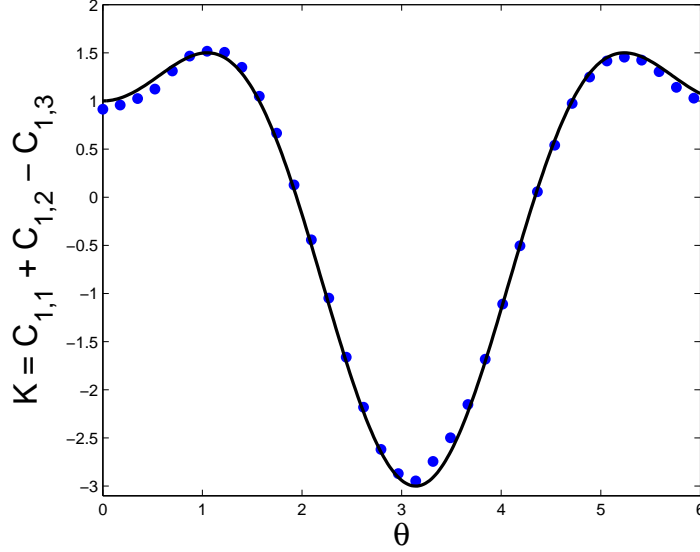
**Figure 2.** Quantum scattering circuit for measuring time correlation functions  $\langle\mathcal{O}(t_m)\mathcal{O}(t_k)\rangle$ , at instants  $t_m$  and  $t_k$  where  $h$  stands for  $H/\hbar$ . The correlation can be obtained by measuring the expected value  $\langle\sigma_z\rangle$  of the ancillary qubit.



**Figure 3.** Experimental tomographed input deviation density matrix  $\Delta\rho = |0\rangle\langle 0| \otimes \mathcal{I}/2 - \mathcal{I}/4$ . The fidelity between the experimental and theoretical matrices is  $\approx 0.99$ .



**Figure 4.** Correlation functions obtained in three different experiments. With extra ancillary qubits it is possible to measure them all in a single run. The x-axis corresponds to a full  $2\pi$  cycle;  $\theta$  stands for  $\Delta E \Delta t / \hbar$ .



**Figure 5.** Violation of Leggett-Garg inequality, Eq. (1). The x-axis corresponds to a full  $2\pi$  cycle;  $\theta$  stands for  $\Delta E \Delta t / \hbar$ . The maximum violation occurs at  $\pi/3$  and  $5\pi/3$ .

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